Appendix C

NDDH Calpuff

Postprocessing System

Calpuff

Increment Tracking

and

Output Visualization

System

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Overview

The Calpuff Increment Tracking and Output Visualization System (CITOVS) is a postprocessing system intended to aid in the interpretation of Calpuff model results for Class I areas. It includes a component for tracking individual source contributions at fixed Class I receptors, and a component for visualizing predicted cumulative concentration patterns over a broader area encompassing much of western North Dakota. The system can be used to track PSD Class I increments and other air quality related values.

The CITOVS is illustrated in Figure 1. The system incorporates the Calpuff model, the Calpost postprocessor, and several supporting programs which include commercial products and some developed by the North Dakota Department of Health (NDDH). Primary features of CITOVS are the master source concentration file (SCF) and the master grid concentration file (GCF).

The SCF contains the hourly contributions for each source or source group processed with Calpuff at each Class I receptor. Each execution of Calpuff/SRCIN adds a new source layer to the SCF. The SRCOUT program is used to total selected source layer concentrations in the SCF, and provide a resultant file compatible with Calpost. Calpost is then applied in a conventional manner to produce a report summarizing the cumulative impact of selected sources at Class I receptors.

The SCF accommodates 50 fixed Class I area receptors. North Dakota Class I area receptors (44) are depicted in Figure 2. In addition, the SCF includes five receptors for Class I areas in Montana (i.e., Medicine Lake Wilderness Area (1) and Fort Peck Reservation (4)).

The GCF contains the cumulative hourly concentrations for each source or source group processed with Calpuff, for a fixed receptor grid which encompasses all North Dakota Class I areas (Figure 3). This regional receptor grid accommodates visual interpretations of Calpuff model output. Each execution of Calpuff/GRDIN adds to the cumulative concentrations stored in the GCF. Calpost may be subsequently applied to produce a summary report or plot files reflecting the cumulative concentrations stored in the GCF. Likewise, the GRDOUT program can be applied to select an episode from the GCF for animated display, through subsequent application of CALMOVIE and GIF animation software.

The CALXCEED postprocessor was added to compliment Calpost. CALXCEED operates on cumulative source output from SRCOUT to summarize exceedances of a given threshold value at each receptor,

Figure 1
Calpuff Increment Tracking
and
Output Visualization System

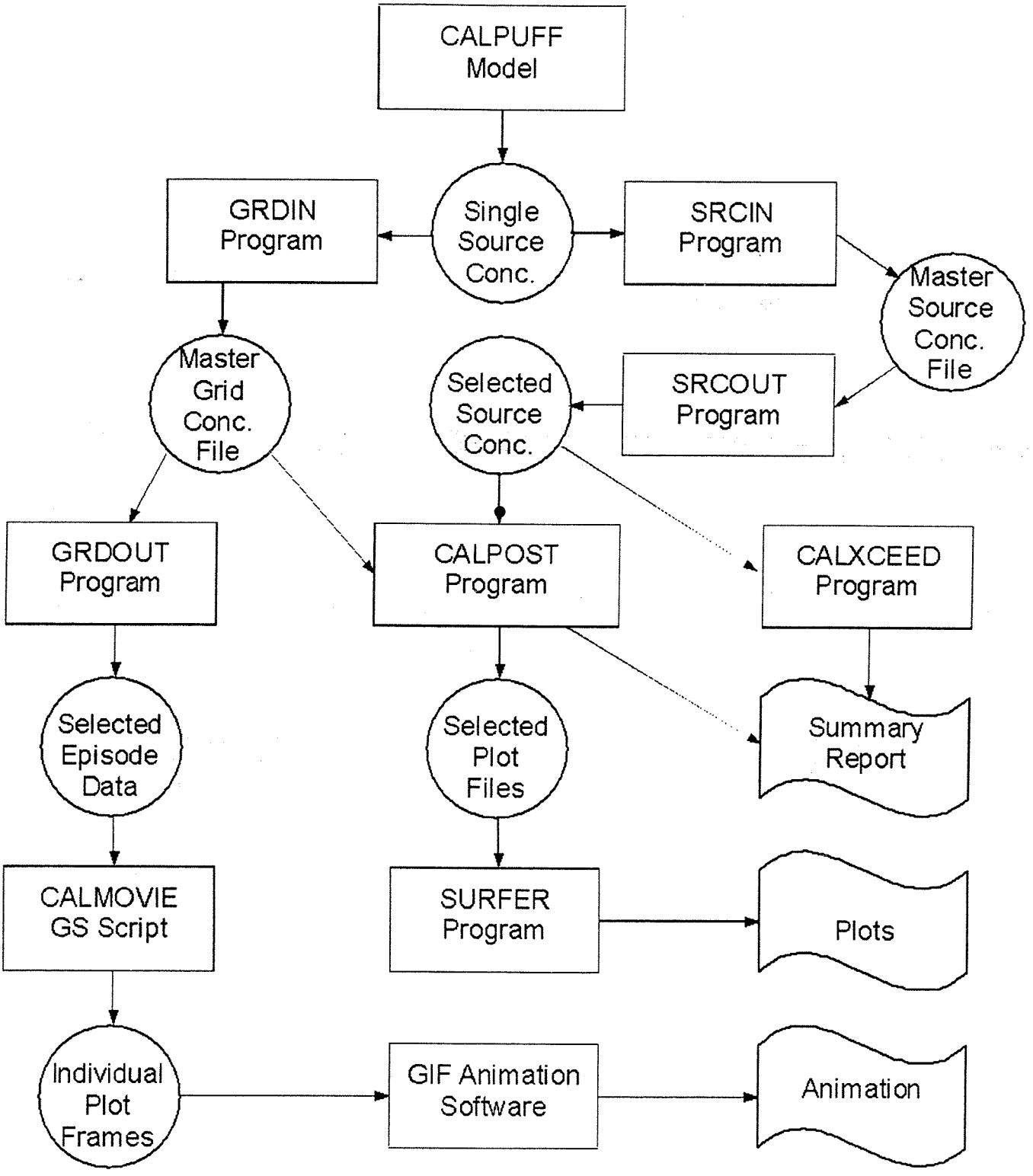


Figure 2
North Dakota Class I Area Receptors

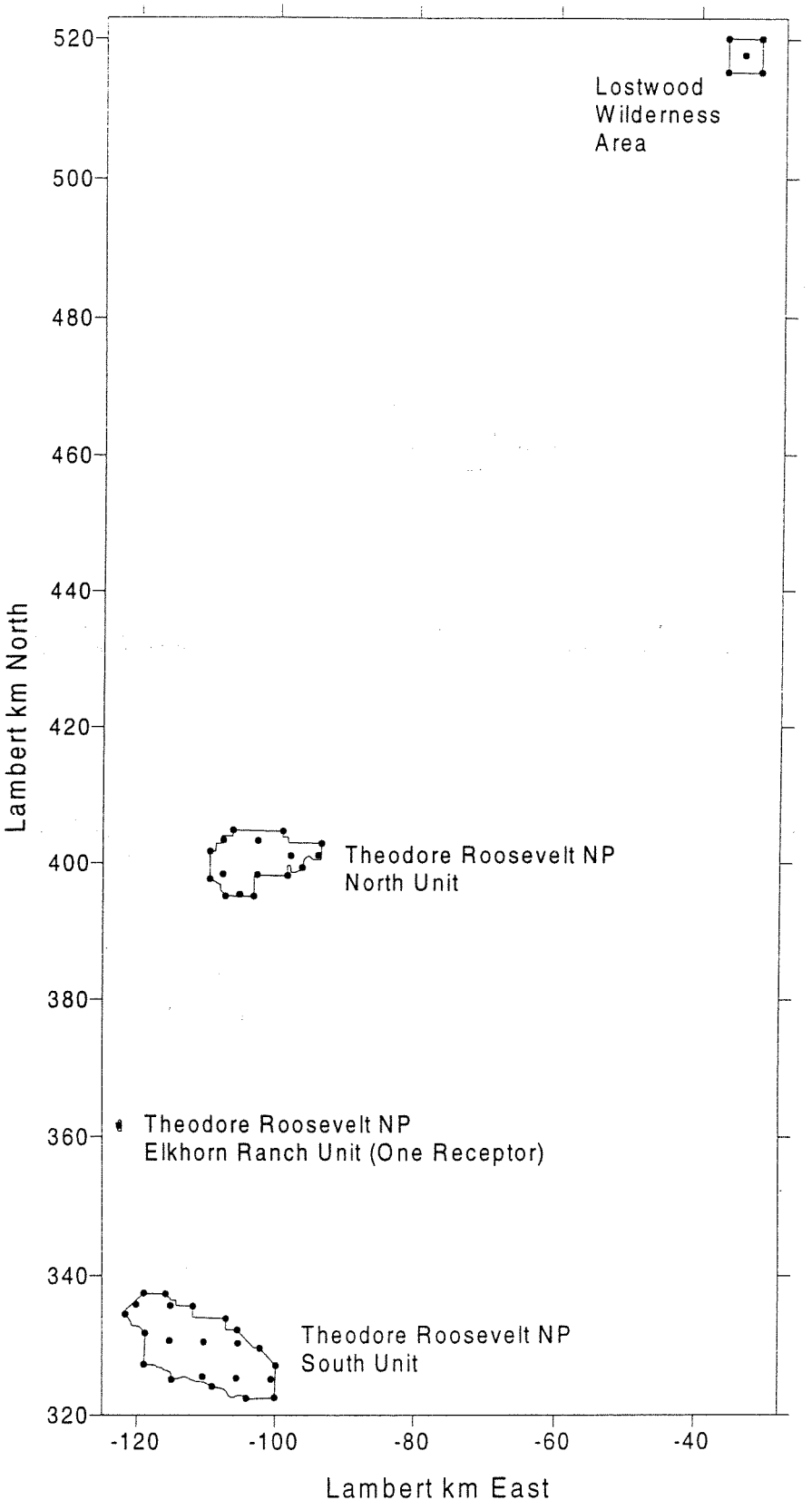
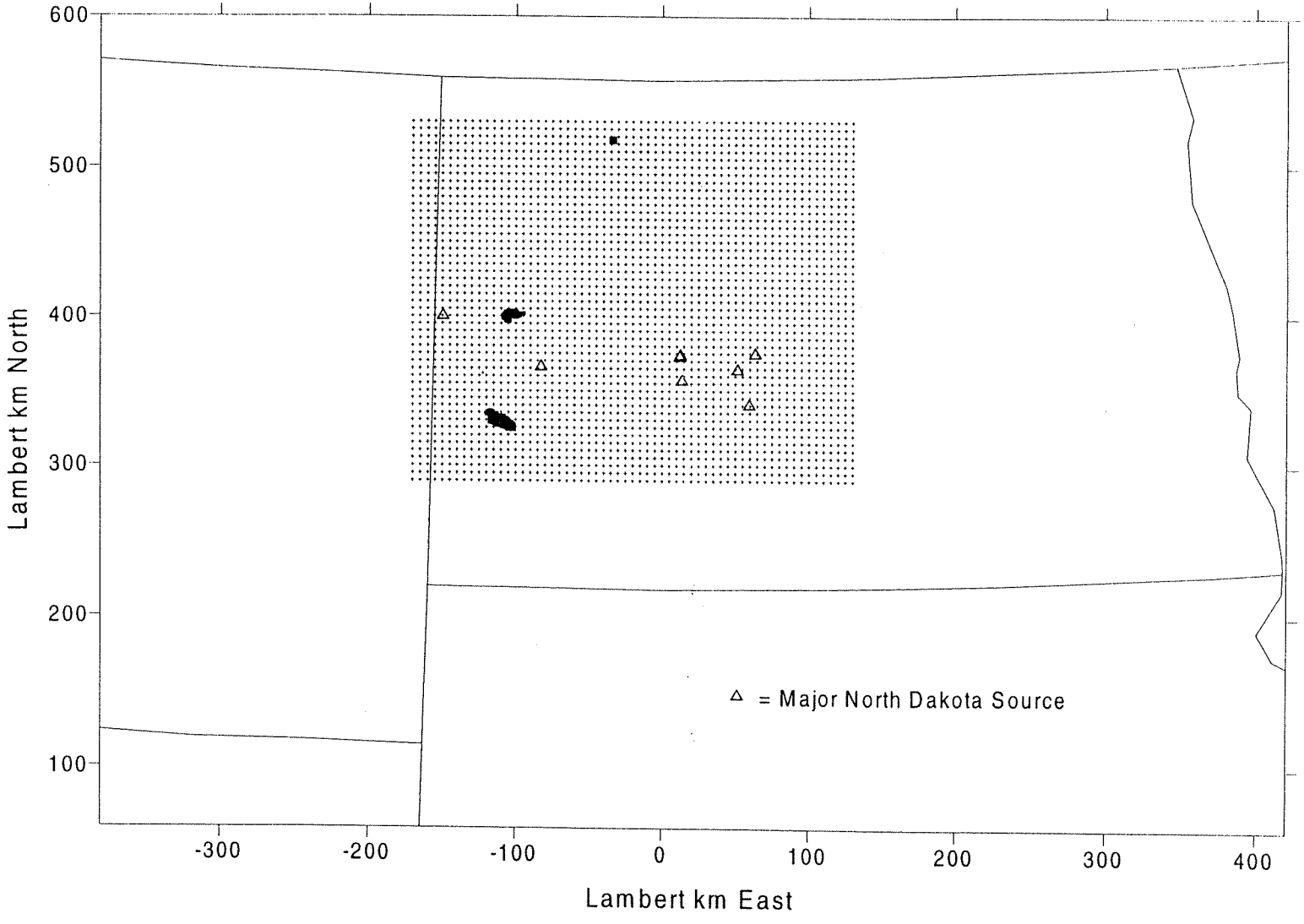


Figure 3
Location of GCF Receptor Grid within Calmet Grid



and provides the contribution of a selected single source to each exceedance.

A primary objective of CITOVS is to simplify Class I modeling procedure by providing a capability for archiving individual source (or source group) concentrations, such that any new regulatory action reduces to modeling new source emissions, only. This system is also more amenable to increment tracking, as the effects (on cumulative predictions) of sources which are modified, or shut down, can more easily be accounted for. One caveat here is that the concept inherent in CITOVS (i.e., modeling and tracking individual source impact) may not be valid if significant chemical interaction among multiple sources is anticipated. The North Dakota Department of Health has conducted considerable sensitivity testing of Calpuff, and found that such chemical interaction which affects model results is rare, and will potentially occur only among very tightly grouped sources. Nevertheless, the user should be aware of this potential limitation.

This report focuses on documentation for the Fortran programs and GS script developed by the NDDH, i.e., SRCIN, SRCOUT, GRDIN, GRDOUT, CALXCEED, and CALMOVIE. Documentation for Calpuff, Calpost, and the commercial program SURFER is available elsewhere.

SRCIN

Purpose: To add Calpuff hourly output from one source or a group of sources to the master source concentration file (SCF). For each source (source group), the SCF contains hourly concentrations for up to six species at all Class I receptors. SCRIN and the SCF also provide capability for tracking PSD-increment-expanding sources, as Calpuff cannot directly accommodate negative emission sources. The SCF is based on a complete year of hourly concentration data, and SCRIN will not accept Calpuff output from less than a full-year run.

Options: SRCIN allows the user to add a new Calpuff source (source group) layer to the SCF, to completely replace an existing layer in the SCF, or to selectively update an existing layer in the SCF. The last option allows updating of the source layer hourly concentrations with respect to any species and receptor, and provides considerable flexibility. For example, the results of a Calpuff run for SO_4 at Theodore Roosevelt National Park (TRNP) North Unit receptors can be added to an existing source layer containing Calpuff output for SO_2 at TRNP south unit receptors. For any option, only those species/receptors contained in the Calpuff output file are affected in the SCF.

For each source layer, the SCF stores concentrations for 50 receptors (all Class I receptors), and for either two or six pollutant species. The latter provision is intended to save disk space. The user can opt to store SO_2/SO_4, NO_x/NO_3, $PM_{10}/PM_{2.5}$, or all six species in the source layer. Once a layer has been established, however, the update option cannot be used to change, or increase the number of, species. Likewise, the replace option cannot increase/decrease the number of species. For example, an SO_2/SO_4 source layer can be replaced with a NO_x/NO_3 source layer, but a SO_2/SO_4 layer cannot be replaced with a layer containing all six species. There is no limit to the number of source layers which can be contained in the SCF.

When the replacement option is selected, concentrations for all species and receptors in the layer are replaced. Concentrations for species or receptors which are not present in the Calpuff output file are set to zero in the SCF. That is, if a SO_2/SO_4 layer is being replaced with a NO_x/NO_3 layer, and only NO_x is included in the Calpuff output file, NO_3 concentrations in the SCF are set to zero.

The Calpuff hourly output file may include gridded receptors or non-Class I area discrete receptors. SRCIN automatically processes

only the discrete Class I receptors (i.e., North Dakota Class I receptor coordinates are hard-coded in the program).

Execution: A control input file is required for execution of SRCIN. The format of the control file is outlined in Table 1. The required name for the control file is SRCIN.CTL.

SRCIN is executed by typing the complete path for the SRCIN executable at the DOS command prompt.

Note that the SRCIN output file (SCF) name is currently hard-coded SRCFILnn.DA, where nn is the two-digit year. The path for this file is entered in Record 3 of the control file (Table 1).

SRCIN expects the year of this file to agree with the year in the Calpuff output file.

As indicated in Table 1, a fourth control file record must be provided if an SCF source layer is to be replaced. This record contains the title of the layer to be replaced. When source layers are initially established (i.e., SRCIN is executed with source layer option 1), SRCIN assumes the first (of three) Calpuff title lines for the title of the source layer, and stores this title in the SCF header. Therefore, care should be exercised in specifying the first title line in the Calpuff input file (source name should be referenced). The title specified for the layer to be replaced by SRCIN must match exactly. Likewise, the title used in the Calpuff input file to update a source layer must exactly match that in the SCF.

Note that Calpuff output for PSD-increment-expanding sources is handled by preceding the selected source layer option (LOPT) in the control file with a minus sign. This causes the Calpuff hourly concentrations to be stored as negative values in the SCF.

SRCIN maintains the current makeup of the SCF in a log file called SRCFILnn.LOG, where nn is the two-digit year. The log file contains a listing of title and species option for each source layer in the SCF. The log file is updated each time SRCIN is executed, and is placed in the same directory as the SCF.

Table 1: SRCIN Control File Inputs (SRCIN.CTL)

Free Format

Record No.	Variable	Type	Description
1	LOPT	int.	Source layer option 1-3 (1 = add new layer, 2 = replace existing layer, 3 = update existing layer, precede with minus sign for increment expanding source, i.e., -2 replaces layer specified in Record 4 with Calpuff output for increment expanding source)
1	ISPOPT	int.	Species option 1-4 (1 = SO_2/SO_4, 2 = NO_x/NO_3, 3 = $PM_{10}/PM_{2.5}$, 4 = All six species)
2	CONFIL	char.	Calpuff concentration file name (complete path)
3	SRCPTH	char.	Source concentration file path* (e.g.,E:\CALPUFF\)
4**	INTITL	char.	Title of layer to be replaced

* If source concentration file not found in path, it will be created.

** Record No. 4 required only if LOPT = 2.

SRCOUT

Purpose: To sum hourly concentrations from more than one source layer in the master source concentration file (SCF), and store the results in a Calpuff-compatible output file for subsequent processing with Calpost. SRCOUT extracts hourly data for a full year.

Options: SRCOUT is an interactive program which allows the user to select the species, source layers, and receptors (in the SCF) to be processed for use with Calpost or CALXCEED. Species are selected from SO_2/SO_4, NO_x/NO_3, or $PM_{10}/PM_{2.5}$. The user has the option of selecting all source layers which match the selected species, or selecting source layers individually. Receptors may be selected in total, or on the basis of individual Class I areas.

Execution: SRCOUT is an interactive program which prompts the user for all necessary input information. SRCOUT is executed by typing the complete path for the SRCOUT executable at the DOS command prompt, followed by the complete path for the SCF name. For example,

```
C:\>SRCOUT    G:\SRCFIL90.DA
```

the Calpost-compatible output is written to file CALPUFnn.CON where nn is the two-digit year.

GRDIN

Purpose: To add (subtract) Calpuff hourly output from one source or a group of sources to the master grid concentration file (GCF). The GCF maintains a cumulative total of hourly concentrations for all Calpuff hourly output files processed with GRDIN. The GCF is based on a fixed receptor grid, four fixed species (SO_2, SO_4, NO_x, NO_3) and a complete year of hourly concentration data. GRDIN will not accept Calpuff output from less than a full-year run. The GCF has the same format as the Calpuff hourly output file, and thus is compatible for direct processing with Calpost.

Options: GRDIN allows the user to add Calpuff output hourly concentrations for a new source (source group) to the GCF or to subtract Calpuff output hourly concentrations for a source (source group) which is already included in the GCF total. There is no species selection option. Concentrations for whichever of the four species SO_2, SO_4, NO_x, NO_3 that are present in the Calpuff output file will be added to (subtracted from) the GCF cumulative total for those species. For any of these four species which are not present in the Calpuff output file, no change is made to the GCF. The receptor grid in the Calpuff hourly output file must match the fixed grid in the GCF. Discrete receptors in the Calpuff hourly output file are ignored by GRDIN.

There is no limit to the number of sources (source groups) which can be added to the GCF. Because the GCF tracks cumulative concentrations only, the addition/deletion of sources does not change the file size.

Execution: A control input file is required for execution of GRDIN. The format of the control file is outlined in Table 2. The required name for the control file is GRDIN.CTL. GRDIN is executed by typing the complete path for the GRDIN executable at the DOS command prompt.

Note that the GRDIN output file (GCF) name is currently hard-coded GRDFILnn.DAT, where nn is the two-digit year. The path for this file is entered in Record 3 of the control file (Table 2). If the GCF does not exist, it will be created.

Because the GCF is a sequential file, the original file cannot be selectively modified. Therefore, the GCF modification as a result of GRDIN activity is placed in a new output file named GRDFILnn.DA2 (same directory). The user must delete the old file and rename the new before subsequent GRDIN application.

Table 2: GRDIN Control File Inputs (GRDIN.CTL)

Free format

Record No.	Variable	Type	Description
1	ICOPT	int.	Concentration option 1-2 (1 = add Calpuff conc. to grid conc. file, 2 = subtract Calpuff conc. from grid conc. file)
2	CONFIL	char.	Calpuff concentration file name (complete path)
3	GRDPTH	char.	Grid concentration file path* (e.g.,E:\CALPUFF\)

* If grid concentration file not found in path, it will be created.

GRDIN maintains the current makeup of the GCF in a log file named GRDFILnn.LOG, where nn is the two-digit year. The log file contains a listing of title and species for each source (source group) accounted for in the GCF. Note that the first of three Calpuff title lines is used as the source title. When exercising the option to subtract a source contribution from the GCF, the first Calpuff title line must exactly match (first 50 characters) a title in the GCF log file. The log file is placed in the same directory as the GCF.

GRDOUT

Purpose: To extract hourly concentration data from the master grid concentration file (GCF) and produce a sequence of concentration XYZ file(s) to facilitate the preparation of plots using SURFER, or animated movies using CALMOVIE. Because the GCF uses the same format as the Calpuff hourly output file, GRDOUT will also work with any Calpuff hourly output file (GRDOUT is not currently compatible with Calpuff output which includes discrete receptors). As an option, concurrent data can be extracted from the Calmet meteorological data file and a post file prepared so that wind vectors and mixing heights can be overlaid on concentration plots/movies.

Options: GRDOUT is an interactive program which allows the user to select the period and species (SO_2, SO_4, NO_x, NO_3) to be processed into hourly XYZ files. The option to prepare hourly posting files for wind vectors and mixing heights is also available. Wind vectors are included for the first five Calmet layers. These hourly XYZ and post files are concatenated into single files (i.e., one XYZ file, one post file) which include interleaving header records for compatibility with CALMOVIE. If these files are to be used with SURFER in a conventional sense, the hourly components must be separated and header records removed.

Execution: GRDOUT is an interactive program which prompts the user for all necessary input information. GRDOUT is executed by typing the complete path for the GRDOUT executable at the DOS command prompt, followed by the complete path for the GCF/Calpuff output file name. For example,

```
C:\>GRDOUT    G:\GRDFIL90.DAT
```

If the option to prepare a meteorological data (wind-vector) post file is selected, the user will be prompted for a Calmet-compatible file name (complete path). The XYZ (concentration) output is written to file XYZFIL and the post (meteorological data) output is written to file PSTFIL.

CALMOVIE

Purpose: GS (Golden Software) script which works with XYZ and post file output from GRDOUT to produce a sequence of hourly plot frames in image file (gif) format. Animation software (such as GIF Construction Set) can be subsequently applied to produce an animated move of hourly concentration patterns.

Options: This interactive script presents the user with several options for enhancing the basic contour plot. These include:

1) Add a title
2) Overlay meteorological data (wind vectors and mixing heights)
3) Overlay background map (county boundaries and selected cities)
4) Post source locations

The size of the plot frame is governed by the limits of data points in the XYZ file. If the option to overlay meteorological data is selected, the user will be prompted to select a wind layer between 1 and 5 (wind data for first five Calmet layers is stored in post file). The wind vector (size proportional to wind speed) and mixing height (ten's of meters) is displayed for each Calmet grid cell. Source locations are obtained from a post file which must be prepared by the user.

Installation: Installation is accomplished by copying all of the files included with the CALMOVIE distribution into directory:

C:\Surfer6\Script

The files needed for the CALMOVIE system, including the distribution files, are described in Table 3.

Execution: CALMOVIE is executed by first launching GS Scriptor, then opening CALMOVIE from the GS Scripter file menu, and finally selecting 'start' from the GS Scripter run menu. The user will be prompted for options as described above. The user is also prompted for the path (directory) where the XYZ and post (met data) files are located, and for the path (directory) where image output files are to be stored.

Source locations may be posted using the information in file SRCLAM.DAT, which is located in directory:

C:\Surfer6\Script

This file must be prepared by the user, and its format is shown in Table 4.

Table 3: CALMOVIE Files

File Name	Type	Description
Files included with CALMOVIE distribution:		
CALMOVIE.BAS	GS Script	CALMOVIE script file
TRSULAM.BLN	input	Boundary line file for T.R. South Unit Class I area
TRNULAM.BLN	input	Boundary line file for T.R. North Unit Class I area
TRELKLAM.BLN	input	Boundary line file for T.R., Elkhorn Ranch Class I area
LOSTLAM.BLN	input	Boundary line file for Lostwood Class I area
COUNTLAM.BLN	input	Boundary line file for ND counties
CITYLAM.DAT	input	Post file for ND cities
CALPUFF.LVL	input	Concentration contour level file
Other CALMOVIE files:		
XYZFIL	input	XYZ file of hourly concentrations from GRDOUT
PSTFIL	input	Met. data post file from GRDOUT
SRCLAM.DAT	input	Source location post file (user-prepared)
XXXXXX.GIF	output	Hourly concentration image file*

* One image (file) is generated for each hour of episode selected in GRDOUT. Image files are named sequentially starting with 1000.GIF.

Table 4: Source Location Posting File (SRCLAM.DAT)

Free Format

Record No.*	Variable	Type	Description
1	X	real	X-coordinate in Lambert Km
1	Y	real	Y-coordinate in Lambert Km
1	LABEL	char.	Source name enclosed in double quotes

* One record needed for each source.

CALXCEED

Purpose: To summarize Calpuff-predicted exceedances of given threshold values (usually PSD Class I increments). CALXCEED is intended to operate on cumulative source output from SRCOUT, but is also compatible for direct processing of Calpuff hourly output. CALXCEED was developed to compliment Calpost by providing additional information on exceedances. While Calpost provides the number of exceedances of user-selected threshold values, CALXCEED lists the value, location, and time of each predicted exceedance. CALXCEED also provides the contribution of a selected single source to each exceedance.

Options: The current version of CALXCEED provides no options and requires no user input. Threshold values are hard-coded as SO_2 Class I increments, so the program summarizes exceedances of Class I increments for SO_2, only. It is anticipated the program will be expanded to address exceedances of Class I increments for other species, and exceedances of threshold values for other air quality related values.

Execution: A DOS batch file (CALXCEED.BAT) is required for execution of CALXCEED. The command line format includes the batch file name followed by three additional file names:

1) Cumulative SRCOUT/Calpuff output file (complete path)
2) Single-source Calpuff output file (complete path)
3) Output list file

For example:

```
c:>CALXCEED.BAT D:\CUMFILE.dat D:\SINFILE.DAT OUTPUT.LST
```

SFW:csc